



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:07 PM GMT

PDB ID : 4KLC
Title : E343D/F110A Double mutant of human ferrochelatase
Authors : Lanzilotta, W.N.; Medlock, A.E.
Deposited on : 2013-05-07
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

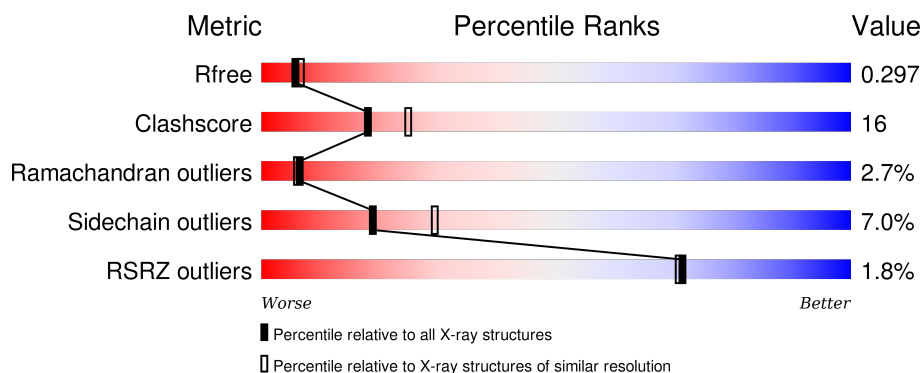
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	370	
1	B	370	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEM	A	502	-	-	-	X
3	HEM	B	503	-	-	-	X
4	GOL	B	502[A]	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6182 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ferrochelatase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2884	1834	503	529	18			
1	B	359	Total	C	N	O	S	0	0	0
			2884	1834	503	529	18			

There are 26 discrepancies between the modelled and reference sequences:

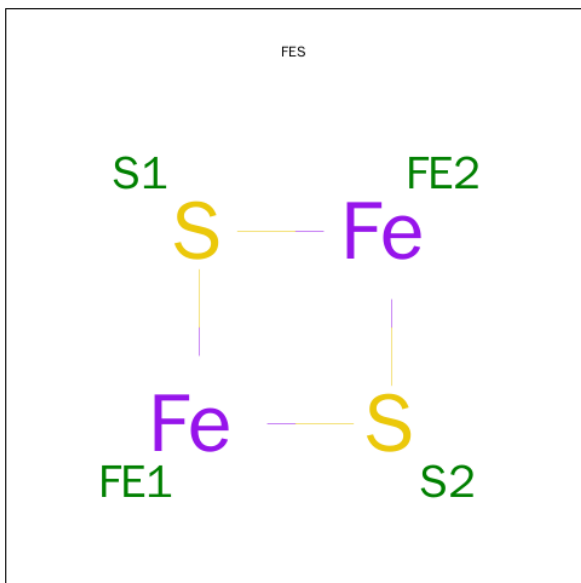
Chain	Residue	Modelled	Actual	Comment	Reference
A	54	MET	-	EXPRESSION TAG	UNP P22830
A	55	GLY	-	EXPRESSION TAG	UNP P22830
A	56	GLY	-	EXPRESSION TAG	UNP P22830
A	57	SER	-	EXPRESSION TAG	UNP P22830
A	58	HIS	-	EXPRESSION TAG	UNP P22830
A	59	HIS	-	EXPRESSION TAG	UNP P22830
A	60	HIS	-	EXPRESSION TAG	UNP P22830
A	61	HIS	-	EXPRESSION TAG	UNP P22830
A	62	HIS	-	EXPRESSION TAG	UNP P22830
A	63	HIS	-	EXPRESSION TAG	UNP P22830
A	64	GLY	-	EXPRESSION TAG	UNP P22830
A	110	ALA	PHE	ENGINEERED MUTATION	UNP P22830
A	343	ASP	GLU	ENGINEERED MUTATION	UNP P22830
B	54	MET	-	EXPRESSION TAG	UNP P22830
B	55	GLY	-	EXPRESSION TAG	UNP P22830
B	56	GLY	-	EXPRESSION TAG	UNP P22830
B	57	SER	-	EXPRESSION TAG	UNP P22830
B	58	HIS	-	EXPRESSION TAG	UNP P22830
B	59	HIS	-	EXPRESSION TAG	UNP P22830
B	60	HIS	-	EXPRESSION TAG	UNP P22830
B	61	HIS	-	EXPRESSION TAG	UNP P22830
B	62	HIS	-	EXPRESSION TAG	UNP P22830
B	63	HIS	-	EXPRESSION TAG	UNP P22830
B	64	GLY	-	EXPRESSION TAG	UNP P22830
B	110	ALA	PHE	ENGINEERED MUTATION	UNP P22830

Continued on next page...

Continued from previous page...

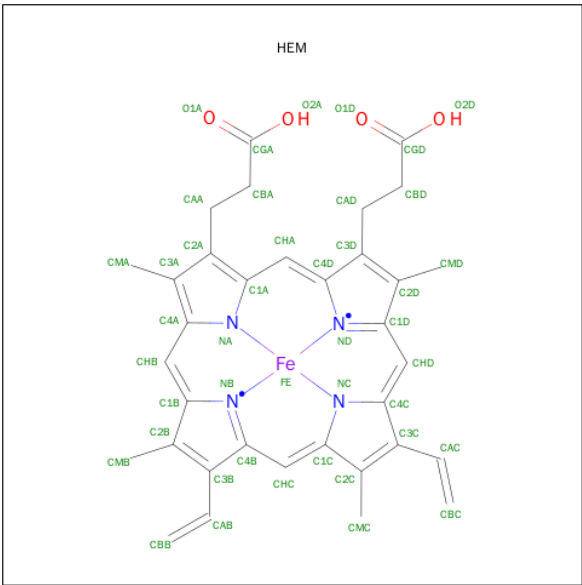
Chain	Residue	Modelled	Actual	Comment	Reference
B	343	ASP	GLU	ENGINEERED MUTATION	UNP P22830

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



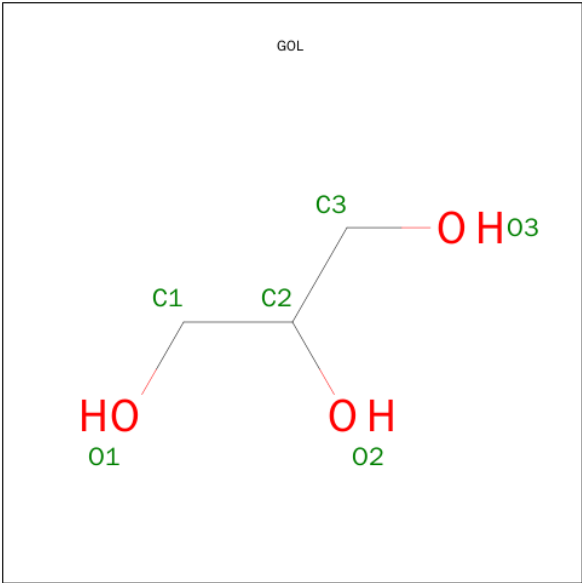
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	1
			12	6	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total 173	O 173	0	0
5	B	135	Total 135	O 135	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	62.66 Å 133.40 Å 136.78 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	136.78 – 2.40 46.20 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (136.78-2.40) 97.8 (46.20-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.255 , 0.299 0.254 , 0.297	Depositor DCC
R_{free} test set	2254 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.6	EDS
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	3 of 44854 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6182	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 79.43 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.5885e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FES, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	0/2953	0.91	6/4001 (0.1%)
1	B	0.86	0/2953	0.88	6/4001 (0.1%)
All	All	0.88	0/5906	0.89	12/8002 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	290	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	B	226	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	290	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	148	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	348	LEU	CA-CB-CG	5.47	127.88	115.30
1	B	298	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	A	316	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	155	ALA	N-CA-C	5.19	125.01	111.00
1	A	343	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	147	LEU	CA-CB-CG	5.17	127.20	115.30
1	B	259	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	107	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	154	THR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2884	0	2893	102	0
1	B	2884	0	2893	84	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	43	0	30	10	0
3	B	43	0	30	9	0
4	B	12	0	16	5	0
5	A	173	0	0	9	1
5	B	135	0	0	2	1
All	All	6182	0	5862	184	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PRO:O	1:A:155:ALA:HB2	1.50	1.10
1:A:290:ARG:CG	1:A:290:ARG:HH11	1.66	1.09
1:A:234:ILE:HG13	1:A:286:LYS:HD2	1.11	1.06
1:A:290:ARG:HG2	1:A:290:ARG:NH1	1.66	1.02
1:B:341:HIS:CE1	3:B:503:HEM:HMD3	1.96	1.00
1:A:290:ARG:HG2	1:A:290:ARG:HH11	0.83	0.98
1:A:234:ILE:HG13	1:A:286:LYS:CD	1.93	0.97
1:B:155:ALA:HB1	1:B:156:PRO:CD	1.96	0.96
1:A:277:PRO:HB2	4:B:502[A]:GOL:H2	1.43	0.96
1:A:104:GLN:HA	1:A:107:LEU:HB3	1.47	0.94
1:A:68:LYS:HG3	1:A:156:PRO:HD2	1.50	0.94
1:A:234:ILE:HG21	1:A:286:LYS:HD3	1.52	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ALA:HB1	1:B:156:PRO:HD2	1.51	0.91
1:B:68:LYS:HE2	1:B:155:ALA:HB2	1.50	0.90
1:B:341:HIS:HE1	3:B:503:HEM:HMD3	1.37	0.86
1:B:68:LYS:HE2	1:B:155:ALA:CB	2.07	0.83
1:A:273:GLY:O	1:B:298:ARG:NH1	2.13	0.82
1:A:244:GLU:HG2	5:A:656:HOH:O	1.79	0.81
1:B:101:LEU:C	1:B:103:ILE:H	1.86	0.78
1:B:341:HIS:CE1	3:B:503:HEM:CMD	2.66	0.78
1:A:100:THR:O	1:A:102:PRO:HD3	1.83	0.77
1:B:276:TYR:HB3	1:B:277:PRO:HD3	1.64	0.77
1:B:350:ILE:O	1:B:351:GLU:HB3	1.84	0.76
1:A:152:PRO:O	1:A:155:ALA:CB	2.32	0.76
1:B:352:TYR:O	1:B:357:ALA:HB2	1.85	0.76
1:B:155:ALA:CB	1:B:156:PRO:CD	2.65	0.75
1:A:277:PRO:HB2	4:B:502[A]:GOL:C2	2.17	0.74
1:A:68:LYS:HG3	1:A:156:PRO:CD	2.18	0.74
1:A:296:PRO:HD3	1:B:397:LYS:HD2	1.69	0.73
1:B:68:LYS:CE	1:B:155:ALA:HB2	2.19	0.72
1:A:349:ASP:O	1:A:353:SER:HB2	1.90	0.71
1:A:141:GLU:OE1	5:A:716:HOH:O	2.09	0.70
1:A:252:LYS:HB3	1:A:329:ASN:ND2	2.08	0.69
1:B:76:MET:HG2	1:B:165:TYR:HE1	1.56	0.69
1:A:104:GLN:O	1:A:106:LYS:N	2.22	0.68
1:B:155:ALA:CB	1:B:156:PRO:HD2	2.21	0.68
1:A:415:LYS:HE3	5:A:761:HOH:O	1.93	0.67
1:A:290:ARG:CG	1:A:290:ARG:NH1	2.35	0.67
1:A:263:HIS:CD2	3:A:502:HEM:C4C	2.82	0.67
1:A:116:THR:N	1:A:117:PRO:HD2	2.10	0.67
1:B:316:ASP:HB3	1:B:352:TYR:CE1	2.30	0.67
1:A:335:ILE:HG13	1:A:335:ILE:O	1.94	0.66
1:A:323:CYS:SG	1:A:362:VAL:HG22	2.36	0.66
1:B:350:ILE:O	1:B:351:GLU:CB	2.44	0.65
1:B:76:MET:HG2	1:B:165:TYR:CE1	2.32	0.64
1:A:350:ILE:HA	1:A:354:GLN:OE1	1.98	0.63
1:A:300:VAL:HG12	1:A:313:PRO:HG2	1.81	0.63
1:A:343:ASP:OD1	5:A:750:HOH:O	2.16	0.63
1:A:244:GLU:HG3	1:A:368:ALA:HA	1.80	0.63
1:B:226:ARG:HD3	1:B:279:GLU:OE2	1.99	0.63
1:A:235:GLN:HG3	1:A:290:ARG:HH22	1.65	0.62
1:A:342:ILE:HG22	3:A:502:HEM:CAD	2.30	0.61
1:A:304:LYS:HG2	1:A:304:LYS:O	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ARG:NH2	1:B:410:VAL:HG21	2.15	0.61
1:A:298:ARG:HG3	5:A:692:HOH:O	2.01	0.61
1:B:101:LEU:C	1:B:103:ILE:N	2.53	0.60
1:B:319:ILE:HD11	1:B:332:LEU:HD21	1.83	0.60
1:B:281:SER:OG	4:B:502[B]:GOL:H31	2.01	0.60
1:B:101:LEU:O	1:B:103:ILE:N	2.35	0.60
1:B:182:LEU:HB2	1:B:219:MET:HE2	1.82	0.60
1:A:103:ILE:O	1:A:104:GLN:O	2.20	0.60
3:A:502:HEM:HHD	3:A:502:HEM:HBC2	1.85	0.59
1:A:74:LEU:HD22	1:A:202:SER:HB3	1.84	0.59
1:B:213:VAL:HG13	1:B:215:ARG:HG2	1.84	0.59
1:A:346:TYR:O	1:A:350:ILE:O	2.20	0.59
1:B:75:ASN:OD1	1:B:132:ILE:HD11	2.03	0.59
1:B:101:LEU:HD22	1:B:101:LEU:O	2.03	0.59
1:A:220:LYS:HE3	1:A:423:LEU:O	2.03	0.58
1:B:365:ILE:HG23	1:B:365:ILE:O	2.04	0.58
1:A:342:ILE:HG22	3:A:502:HEM:HAD1	1.86	0.58
1:B:195:SER:HB2	1:B:276:TYR:HB2	1.87	0.57
1:B:105:ASN:C	1:B:107:LEU:H	2.08	0.57
1:A:68:LYS:HG3	1:A:156:PRO:CG	2.36	0.56
1:B:320:LYS:HG2	1:B:360:CYS:SG	2.45	0.56
1:B:208:ARG:HH21	1:B:410:VAL:HG21	1.71	0.56
1:A:332:LEU:HD11	1:A:365:ILE:HD11	1.87	0.56
1:A:232:LEU:HD13	1:A:379:LYS:HG2	1.87	0.55
1:A:68:LYS:HG3	1:A:156:PRO:HG2	1.88	0.55
1:B:341:HIS:CE1	1:B:343:ASP:HB2	2.41	0.55
1:A:231:HIS:HD2	5:A:623:HOH:O	1.90	0.55
1:B:266:PRO:HD2	3:B:503:HEM:HAB	1.89	0.54
1:B:68:LYS:HB3	1:B:155:ALA:HB3	1.90	0.54
1:A:104:GLN:HG3	1:A:105:ASN:H	1.73	0.54
1:B:125:ARG:HA	1:B:125:ARG:CZ	2.38	0.54
1:A:68:LYS:CG	1:A:156:PRO:HD2	2.33	0.54
1:B:122:GLN:NE2	1:B:346:TYR:CE2	2.77	0.53
1:B:122:GLN:HE21	1:B:346:TYR:HD2	1.48	0.53
1:A:252:LYS:HB3	1:A:329:ASN:HD22	1.72	0.53
1:B:207:TYR:CE1	1:B:413:GLU:HG3	2.44	0.53
1:A:337:PHE:HB2	5:A:759:HOH:O	2.09	0.52
1:A:341:HIS:HB2	3:A:502:HEM:O2D	2.10	0.52
1:B:99:MET:O	1:B:102:PRO:HD2	2.10	0.51
1:B:263:HIS:HD2	3:B:503:HEM:C1D	2.29	0.51
1:B:177:MET:HB3	1:B:219:MET:HE1	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLU:N	1:A:251:GLU:OE2	2.38	0.51
1:B:263:HIS:CD2	3:B:503:HEM:C1D	2.99	0.50
1:A:323:CYS:C	1:A:325:ARG:H	2.14	0.50
1:B:104:GLN:HA	1:B:104:GLN:OE1	2.11	0.50
1:B:346:TYR:O	1:B:350:ILE:O	2.30	0.50
1:A:235:GLN:HG3	1:A:290:ARG:NH2	2.27	0.49
1:A:230:HIS:NE2	1:A:383:ASP:OD2	2.43	0.49
1:A:278:GLN:HG2	1:B:281:SER:HB3	1.94	0.49
1:A:182:LEU:HB2	1:A:219:MET:HE2	1.94	0.49
1:B:193:GLN:HG2	1:B:280:VAL:HA	1.94	0.49
1:B:68:LYS:HE2	1:B:155:ALA:HB3	1.94	0.49
1:B:75:ASN:O	1:B:163:PHE:HA	2.13	0.49
1:A:320:LYS:O	1:A:324:GLU:HG3	2.13	0.49
1:B:305:VAL:HG11	3:B:503:HEM:HMA2	1.93	0.49
1:A:100:THR:C	1:A:102:PRO:HD3	2.32	0.49
1:A:320:LYS:O	1:A:320:LYS:HG2	2.12	0.48
1:A:342:ILE:HG22	3:A:502:HEM:HAD2	1.96	0.48
1:A:182:LEU:HB2	1:A:219:MET:CE	2.42	0.48
1:A:76:MET:HA	1:A:164:ARG:HB3	1.96	0.48
1:B:155:ALA:HB1	1:B:156:PRO:HD3	1.93	0.48
1:B:110:ALA:O	1:B:114:ARG:HB2	2.13	0.47
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.95	0.47
1:B:106:LYS:HE3	1:B:106:LYS:H	1.79	0.47
1:A:409:PRO:HA	5:A:733:HOH:O	2.14	0.47
1:A:236:CYS:HB3	1:A:371:LEU:HD22	1.95	0.47
1:B:106:LYS:HA	1:B:109:PRO:HD2	1.96	0.47
1:A:301:TRP:O	1:A:314:GLN:HA	2.14	0.47
1:B:272:ARG:HG2	1:B:272:ARG:O	2.14	0.47
1:A:263:HIS:CD2	3:A:502:HEM:CHD	2.98	0.47
1:B:91:ARG:NH2	5:B:713:HOH:O	2.47	0.47
1:A:277:PRO:HB2	4:B:502[A]:GOL:C3	2.45	0.47
1:B:76:MET:HB2	1:B:191:TYR:OH	2.15	0.47
1:A:175:GLU:OE1	1:A:179:ARG:NH1	2.48	0.46
1:B:349:ASP:O	1:B:353:SER:HB2	2.15	0.46
1:A:152:PRO:C	1:A:155:ALA:HB2	2.30	0.46
3:B:503:HEM:HBD1	3:B:503:HEM:HHA	1.98	0.46
1:B:407:VAL:O	1:B:409:PRO:HD3	2.15	0.45
1:A:354:GLN:O	1:A:358:LYS:HB2	2.16	0.45
1:A:102:PRO:O	1:A:103:ILE:HG22	2.16	0.45
1:A:274:ASP:HA	1:A:275:PRO:HD3	1.82	0.45
1:A:263:HIS:CD2	3:A:502:HEM:C1D	3.04	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:PRO:HB2	4:B:502[A]:GOL:H32	1.99	0.45
1:B:87:ASP:OD1	1:B:91:ARG:CZ	2.65	0.45
1:A:328:LYS:HD2	1:A:361:GLY:O	2.17	0.45
1:B:97:ASP:HB2	1:B:201:SER:OG	2.17	0.45
1:B:262:ALA:HB1	1:B:276:TYR:OH	2.17	0.44
1:A:337:PHE:CE1	3:A:502:HEM:HMD1	2.52	0.44
1:A:124:ARG:HG2	1:A:125:ARG:HH21	1.81	0.44
1:A:323:CYS:C	1:A:325:ARG:N	2.71	0.44
1:A:332:LEU:HB2	1:A:367:ARG:HG2	1.99	0.44
1:A:103:ILE:O	1:A:103:ILE:HG13	2.18	0.44
1:A:104:GLN:HG3	1:A:105:ASN:N	2.33	0.44
1:B:312:GLY:HA2	1:B:313:PRO:O	2.18	0.43
1:A:304:LYS:CG	1:A:304:LYS:O	2.65	0.43
1:A:337:PHE:CE1	3:A:502:HEM:CMD	3.02	0.43
1:A:304:LYS:HA	1:A:310:TRP:CD2	2.54	0.43
1:A:253:ARG:O	1:A:256:VAL:HG23	2.18	0.43
1:A:264:SER:HB3	1:A:310:TRP:HE3	1.82	0.43
1:B:283:THR:O	1:B:287:VAL:HG23	2.19	0.43
1:B:107:LEU:O	1:B:111:ILE:HG13	2.19	0.43
1:B:398:GLN:OE1	1:B:398:GLN:HA	2.19	0.42
1:A:189:THR:HG23	1:A:189:THR:O	2.18	0.42
1:B:118:LYS:O	1:B:121:GLU:HB2	2.19	0.42
1:A:350:ILE:O	1:A:351:GLU:HB3	2.19	0.42
1:B:314:GLN:HB3	1:B:316:ASP:OD2	2.19	0.42
1:B:308:MET:HB3	1:B:309:PRO:HD2	2.00	0.42
1:A:138:LYS:HD3	1:A:138:LYS:HA	1.81	0.42
1:B:105:ASN:C	1:B:107:LEU:N	2.73	0.42
1:B:149:GLU:HA	5:B:729:HOH:O	2.19	0.42
1:A:273:GLY:HA2	1:B:313:PRO:CG	2.49	0.42
1:B:408:ASN:OD1	1:B:410:VAL:HG23	2.19	0.42
1:A:76:MET:HB2	1:A:165:TYR:CD1	2.55	0.42
1:A:132:ILE:HG23	1:A:133:LYS:N	2.34	0.42
1:A:196:CYS:SG	5:A:762:HOH:O	2.62	0.42
1:A:234:ILE:HG21	1:A:286:LYS:CD	2.37	0.42
1:B:102:PRO:HB3	1:B:105:ASN:OD1	2.20	0.41
1:B:89:LEU:HD11	1:B:119:ILE:HG13	2.02	0.41
1:A:193:GLN:OE1	1:A:336:ALA:HA	2.20	0.41
1:A:323:CYS:O	1:A:325:ARG:N	2.53	0.41
1:A:231:HIS:H	1:A:231:HIS:CD2	2.39	0.41
1:B:263:HIS:CD2	3:B:503:HEM:C4C	3.08	0.41
1:B:122:GLN:O	1:B:125:ARG:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ARG:HA	1:A:415:LYS:HE2	2.03	0.41
1:A:92:LEU:C	1:A:92:LEU:HD23	2.41	0.41
1:B:75:ASN:CG	1:B:132:ILE:HD11	2.40	0.41
1:A:178:GLU:OE2	1:A:210:TYR:CE2	2.74	0.41
1:A:68:LYS:HE3	1:A:68:LYS:HB3	1.82	0.40
1:B:248:PHE:CZ	1:B:366:ARG:HG3	2.56	0.40
1:B:342:ILE:HD13	1:B:346:TYR:HB3	2.02	0.40
1:B:391:SER:OG	1:B:393:GLU:HG2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:729:HOH:O	5:B:730:HOH:O[2_555]	2.08	0.12
5:A:767:HOH:O	5:A:768:HOH:O[2_555]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/370 (96%)	326 (91%)	21 (6%)	10 (3%)	6	5
1	B	357/370 (96%)	317 (89%)	31 (9%)	9 (2%)	7	7
All	All	714/740 (96%)	643 (90%)	52 (7%)	19 (3%)	6	6

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	THR
1	A	104	GLN
1	A	304	LYS
1	B	155	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	355	VAL
1	B	359	GLU
1	B	106	LYS
1	B	351	GLU
1	A	351	GLU
1	A	421	GLN
1	B	357	ALA
1	B	102	PRO
1	B	303	SER
1	A	155	ALA
1	A	227	TRP
1	A	303	SER
1	B	307	PRO
1	A	103	ILE
1	A	101	LEU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/331 (98%)	303 (94%)	20 (6%)	23	35
1	B	323/331 (98%)	298 (92%)	25 (8%)	16	24
All	All	646/662 (98%)	601 (93%)	45 (7%)	19	29

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	90	LEU
1	A	96	ARG
1	A	100	THR
1	A	107	LEU
1	A	170	THR
1	A	175	GLU
1	A	184	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	211	ASN
1	A	257	VAL
1	A	286	LYS
1	A	290	ARG
1	A	298	ARG
1	A	305	VAL
1	A	320	LYS
1	A	337	PHE
1	A	341	HIS
1	A	359	GLU
1	A	367	ARG
1	A	420	SER
1	B	90	LEU
1	B	100	THR
1	B	101	LEU
1	B	105	ASN
1	B	106	LYS
1	B	107	LEU
1	B	113	LYS
1	B	114	ARG
1	B	126	ILE
1	B	137	SER
1	B	175	GLU
1	B	188	PHE
1	B	213	VAL
1	B	216	LYS
1	B	219	MET
1	B	243	LYS
1	B	250	LEU
1	B	251	GLU
1	B	257	VAL
1	B	304	LYS
1	B	314	GLN
1	B	320	LYS
1	B	339	SER
1	B	342	ILE
1	B	358	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	231	HIS
1	A	302	GLN
1	B	263	HIS
1	B	329	ASN
1	B	341	HIS
1	B	354	GLN
1	B	386	HIS
1	B	421	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FES	A	501	1	0,4,4	0.00	-	0,4,4	0.00	-
3	HEM	A	502	1	30,50,50	2.48	8 (26%)	24,82,82	2.26	7 (29%)
2	FES	B	501	1	0,4,4	0.00	-	0,4,4	0.00	-
4	GOL	B	502[A]	-	5,5,5	0.42	0	5,5,5	1.00	0
4	GOL	B	502[B]	-	5,5,5	0.80	0	5,5,5	1.20	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	B	503	1	30,50,50	2.29	9 (30%)	24,82,82	2.64	14 (58%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FES	A	501	1	-	0/0/4/4	0/1/1/1
3	HEM	A	502	1	-	0/10/54/54	0/0/8/8
2	FES	B	501	1	-	0/0/4/4	0/1/1/1
4	GOL	B	502[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	B	502[B]	-	-	0/4/4/4	0/0/0/0
3	HEM	B	503	1	-	0/10/54/54	0/0/8/8

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	HEM	C3B-C4B	-7.40	1.45	1.51
3	B	503	HEM	C3B-C4B	-7.10	1.45	1.51
3	B	503	HEM	C3D-C4D	-5.73	1.44	1.51
3	A	502	HEM	C3D-C4D	-5.12	1.45	1.51
3	A	502	HEM	C2C-C1C	-4.40	1.44	1.52
3	B	503	HEM	C2C-C1C	-3.68	1.45	1.52
3	B	503	HEM	C2B-C1B	-2.27	1.44	1.51
3	B	503	HEM	C2D-C1D	-2.21	1.44	1.51
3	A	502	HEM	C2B-C1B	-2.07	1.45	1.51
3	B	503	HEM	C4C-NC	2.02	1.38	1.36
3	B	503	HEM	C1C-NC	2.12	1.38	1.36
3	A	502	HEM	C1C-NC	2.39	1.38	1.36
3	B	503	HEM	FE-ND	2.61	2.11	1.97
3	A	502	HEM	C4C-NC	2.72	1.39	1.36
3	A	502	HEM	FE-ND	3.05	2.13	1.97
3	B	503	HEM	FE-NC	4.08	2.11	1.95
3	A	502	HEM	FE-NC	5.30	2.16	1.95

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	HEM	CBA-CAA-C2A	-3.83	105.67	112.53
3	B	503	HEM	C3B-CAB-CBB	-3.34	119.33	124.46
3	B	503	HEM	CAA-CBA-CGA	-3.23	106.83	112.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	HEM	CBD-CAD-C3D	-3.13	104.45	113.55
3	B	503	HEM	C3B-C4B-NB	-2.65	106.56	111.63
4	B	502[B]	GOL	O3-C3-C2	-2.27	99.20	110.18
3	A	502	HEM	C3B-C4B-NB	-2.21	107.41	111.63
3	B	503	HEM	C3C-CAC-CBC	-2.09	121.25	124.46
3	B	503	HEM	C2C-C1C-CHC	2.15	126.95	123.68
3	A	502	HEM	CMD-C2D-C3D	2.24	124.28	114.35
3	B	503	HEM	C2D-C3D-C4D	2.60	105.90	101.50
3	B	503	HEM	CMD-C2D-C3D	2.76	126.58	114.35
3	B	503	HEM	C3B-C4B-CHC	3.14	127.58	123.16
3	A	502	HEM	C3B-C4B-CHC	3.14	127.58	123.16
3	A	502	HEM	CMC-C2C-C3C	3.53	125.34	116.53
3	B	503	HEM	CMC-C2C-C3C	3.70	125.77	116.53
3	A	502	HEM	CMB-C2B-C3B	3.76	125.93	116.53
3	B	503	HEM	CAD-C3D-C4D	4.00	126.57	112.47
3	B	503	HEM	CMB-C2B-C3B	4.00	126.52	116.53
3	A	502	HEM	CAD-C3D-C2D	4.63	126.54	113.22
3	A	502	HEM	CAD-C3D-C4D	4.89	129.72	112.47
3	B	503	HEM	CAD-C3D-C2D	4.98	127.52	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	HEM	10	0
4	B	502[A]	GOL	4	0
4	B	502[B]	GOL	1	0
3	B	503	HEM	9	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	359/370 (97%)	-0.30	7 (1%) 70 69	9, 27, 57, 74	4 (1%)
1	B	359/370 (97%)	-0.30	6 (1%) 73 72	10, 29, 62, 76	4 (1%)
All	All	718/740 (97%)	-0.30	13 (1%) 71 71	9, 28, 60, 76	8 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423	LEU	5.5
1	B	423	LEU	4.6
1	A	422	GLN	3.5
1	A	101	LEU	3.5
1	B	101	LEU	3.3
1	B	100	THR	3.0
1	A	307	PRO	2.9
1	B	103	ILE	2.8
1	B	99	MET	2.7
1	A	305	VAL	2.6
1	B	107	LEU	2.5
1	A	359	GLU	2.2
1	A	100	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	HEM	B	503	43/43	0.81	0.38	4.29	36,42,45,46	43
3	HEM	A	502	43/43	0.85	0.33	3.59	19,33,34,35	43
4	GOL	B	502[B]	6/6	0.96	0.20	1.55	18,19,20,20	6
4	GOL	B	502[A]	6/6	0.96	0.20	1.50	18,19,21,21	6
2	FES	A	501	4/4	0.97	0.05	-2.23	24,24,28,29	0
2	FES	B	501	4/4	0.98	0.04	-3.47	29,30,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.